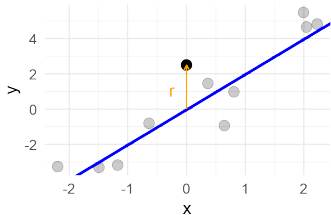


Introduction to Machine Learning

Advanced Risk Minimization Pseudo-Residuals



Learning goals

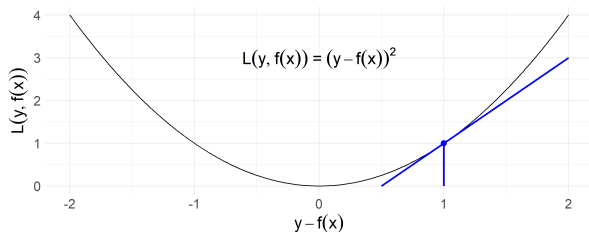
- Concept of pseudo-residuals
- PRs for common losses

PSEUDO-RESIDUALS

- In regression, residuals are defined as $r(\mathbf{x}) := y - f(\mathbf{x})$
- Generalize concept to **pseudo-residuals**:

$$\tilde{r}(\mathbf{x}) := -\frac{dL(y, f(\mathbf{x}))}{df(\mathbf{x})}$$

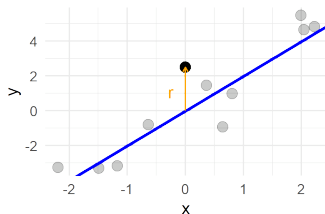
- If we wiggle $f(\mathbf{x})$, how much does L change?
- Can be used for score-based classifiers and other models
- Note that $\tilde{r}(\mathbf{x})$ depends on y , $f(\mathbf{x})$ and L



BEST POINT-WISE UPDATE

- Assume we have (partially) fitted a model $f(\mathbf{x})$ to data \mathcal{D}
- Assume we could update $f(\mathbf{x})$ point-wise as we like
- Under squared loss, for a fixed $\mathbf{x} \in \mathcal{X}$, the best point-wise update is the direction of the residual $r(\mathbf{x}) = y - f(\mathbf{x})$

$$f(\mathbf{x}) \leftarrow f(\mathbf{x}) + r(\mathbf{x})$$

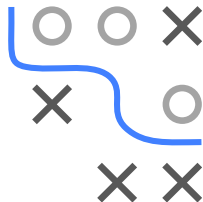
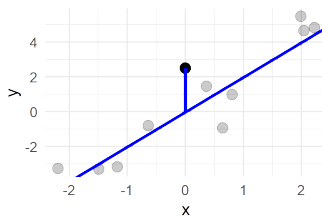


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- Point-wise error at this specific \mathbf{x} becomes 0

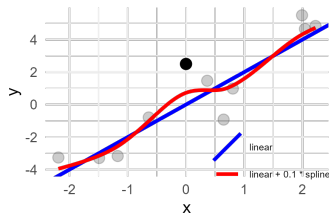
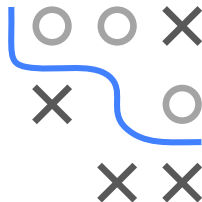


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- (In gradient boosting, which we cover later, we don't do point-wise updates but “smoothly distort” f so we generalize)



APPROXIMATE BEST POINT-WISE UPDATE

- Best local change of f at \mathbf{x} to reduce loss most:

$$f(\mathbf{x}) \leftarrow f(\mathbf{x}) - \frac{dL(y, f(\mathbf{x}))}{df(\mathbf{x})}$$

- This is effectively the PR

$$f(\mathbf{x}) \leftarrow f(\mathbf{x}) + \tilde{r}(\mathbf{x})$$

- (Such iterative updates of f like a loss-reducing GD in function space is the major underlying idea of GB)



GD IN ML AND PSEUDO-RESIDUALS

- In GD, we move in the direction of the negative gradient by updating the parameters:

$$\boldsymbol{\theta}^{[t+1]} = \boldsymbol{\theta}^{[t]} - \alpha^{[t]} \cdot \nabla_{\boldsymbol{\theta}} \mathcal{R}_{\text{emp}}(\boldsymbol{\theta})|_{\boldsymbol{\theta}=\boldsymbol{\theta}^{[t]}}$$

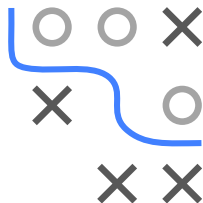
- Using the chain rule:

$$\begin{aligned}\nabla_{\boldsymbol{\theta}} \mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) &= \sum_{i=1}^n \frac{dL(y^{(i)}, f(\mathbf{x}))}{df(\mathbf{x})} \bigg|_{f=f(\mathbf{x}^{(i)} | \boldsymbol{\theta})} \cdot \nabla_{\boldsymbol{\theta}} f(\mathbf{x}^{(i)} | \boldsymbol{\theta}) \\ &= - \sum_{i=1}^n \tilde{r}^{(i)} \cdot \nabla_{\boldsymbol{\theta}} f(\mathbf{x}^{(i)} | \boldsymbol{\theta}).\end{aligned}$$

- Update is loss-optimal directional change of model output and a loss-independent derivative of $f(\mathbf{x})$
- This is a flexible, nearly loss-independent variant of GD



PSEUDO-RESIDUALS FOR COMMON LOSSES



| Loss | Domain of y | Pseudo residual \tilde{r} |
|------------------|-------------------------|----------------------------------------------|
| Squared loss | $y \in \mathbb{R}$ | $y - f(\mathbf{x})$ |
| Bernoulli loss | $y \in \{0, 1\}$ | $y - s(f(\mathbf{x})) = y - \pi(\mathbf{x})$ |
| Multinomial loss | $y \in \{1, \dots, g\}$ | $\mathbb{1}_{\{y=k\}} - \pi_k(\mathbf{x})$ |
| Exponential loss | $y \in \{-1, 1\}$ | $y \exp(-yf(\mathbf{x}))$ |

NB: $\pi(\mathbf{x}) = s(f(\mathbf{x})) = \frac{\exp(f(\mathbf{x}))}{1 + \exp(f(\mathbf{x}))}$ is the (sigmoidal) logistic function, and $\pi_k(\mathbf{x})$ its multi-class generalization, the softmax.